Letters to the Editor

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On the evaluation of effective charge of ionic crystals

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The concept of effective charge occupies a position of central importance in the dielectric theories of ionic crystals. It is, therefore, of practical value to calculate it from theoretical formulae. The shell model due to Dick & Overhauser (1958) has proved itself to be the best upto-date available theory. However, the involvement of so many parameters makes the theory more of a qualitative nature. Hence it is desirable to work on simple formulations for the computation of effective charge. This communication presents such results on some alkali halides which are the proto-type of ionic crystals

Treating the deformation dipole moment, due to overlap between nearest neighbours, in terms of exchange charges, Hardy (1961) showed that the effective charge, s, obeys the relation,

$$1-s = 2d(r_-^{\,2}-r_+^{\,2})(\rho^{-1}-2r_0^{-1})\lambda \exp(-r_0\rho^{-1}). \qquad \ldots \quad (1)$$

The validity of this equation, in the original work, was examined by plotting the experimental values of left hand quantity against the right hand quantities minus the factor $2d$. The relinbility so concluded is of rather approximate nature and the test is rather qualitative. However, the calculation of s from eq. (1) not only leads to theoretical values but their comparison with the experimental data provides a direct and precise check of the appropriateness of the features of the theory also These results are cited in the table. The values of the overlap parameters were obtained through the usual thermodynamical conditions (Born & Mayer 1932). The experimental values are those obtained from Szigeti (1950) relation.

The formulation due to Woods, Cochran & Brockhouse (1960) is of more simplified nature owing to the assumption that only negative ion is polarizable as a consequence of the shell-shell interaction. The final result is

$$\frac{s^2e^2}{\dfrac{3v}{4\pi}A-\left(\dfrac{\epsilon_\infty+2}{\epsilon_\infty-1}\right)e^2(1-s)^2} = \frac{\epsilon_0-1}{\epsilon_0+2}. \qquad \ldots \quad (2)$$

Here we have employed ϵ_0 and ϵ_∞ data of Burstein (1965) except for LiI which